МІНІСТЕРСТВО ОСВІТИ І НАУКИ УКРАЇНИ
СУМСЬКИЙ ДЕРЖАВНИЙ УНІВЕРСИТЕТ

ФІЗИКА, ЕЛЕКТРОНІКА, ЕЛЕКТРОТЕХНІКА

ФЕЕ: 2016

МАТЕРІАЛИ
та програма

НАУКОВО-ТЕХНІЧНОЇ КОНФЕРЕНЦІЇ

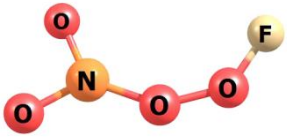
(Суми, 18–22 квітня 2016 року)

Суми
Сумський державний університет
2016

Prototype of Stable Molecular Switch

Anna G. Malashenko[1], *PhD student*; Yuliya A. Shevchenko[1], *student*;
Yuriy M. Lopatkin[1], *professor*; Tatyana N. Sakun[2], *ass. prof.*
[1] Sumy State University, Sumy
[2] National Aviation University, Kiev

One of the goals of molecular electronics is search of structures that can serve as the memory elements, switches, transistors and etc.



As molecular switch may be a molecule which has two conformations, the transition between them is made by an external exposure, for example, the electric field of different polarity. In order to work of element was stable, the molecule must has sufficiently high potential barrier between the two stable states.

As a result of studies, it was found that molecule of nitro peroxide of fluorine (NPF) applies to such molecules. The reversible transition between conformations occurs when an external electric field of 0.035 a.u. As a result, the torsion angle NOOF is changed to 180° (Fig.1).

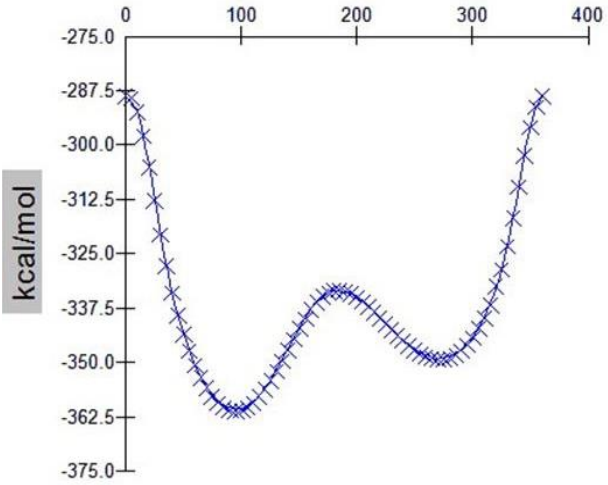


Figure 1 – Dependence of the binding energy of the molecule NPF on the magnitude of the dihedral angle in the external electric field E = 0.035 a.u.

The height of the potential barrier separating these states, greater than 1.5 eV.